The Dynamics of 1D Quantum Spin Systems Can Be Approximated Efficiently

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(Dated: February 1, 2008)

In this Letter we show that an arbitrarily good approximation to the propagator e^{itH} for a 1D lattice of n quantum spins with hamiltonian H may be obtained with polynomial computational resources in n and the error ϵ, and exponential resources in $|t|$. Our proof makes use of the finitely correlated state/matrix product state formalism exploited by numerical renormalisation group algorithms like the density matrix renormalisation group. There are two immediate consequences of this result. The first is that Vidal's time-dependent density matrix renormalisation group will require only polynomial resources to simulate 1D quantum spin systems for logarithmic $|t|$. The second consequence is that continuous-time 1D quantum circuits with logarithmic $|t|$ can be simulated efficiently on a classical computer, despite the fact that, after discretisation, such circuits are of polynomial depth.

The kinematics and dynamics of quantum lattice systems are strongly constrained by a key physical requirement, namely, the *locality of interactions*. For example, consider a collection of n distinguishable spin-$\frac{1}{2}$ systems which interact according to nearest-neighbour interactions: a counting argument quickly reveals that such local hamiltonians occupy an extremely small fraction of the space of general hamiltonians. Thus, intuitively, we would expect this nongeneric constraint would manifest itself strongly in the structure of the eigenvalues and eigenstates for local hamiltonians. This is indeed the case, but it is still far from obvious exactly how to best quantify this constraint.

A number of methods to systematically quantify the eigenstates and matrix functions of local hamiltonians have been developed. Perhaps the most successful scheme in recent years has been the technology of *finitely correlated quantum states* (FCS) [1, 2]. (Finitely correlated states are also known as *matrix product states* (MPS) in one dimension and *tensor product states* or *projected entangled-pair states* in two and higher dimensions [3]. The key feature of a finitely correlated state is that, as the name suggests, separated regions are weakly correlated. In addition, any state which does not exhibit too much correlation between separated subsystems can be well approximated by a finitely correlated state [4], [22].

Finitely correlated states are nothing more than a convenient representation for vectors in tensor-product hilbert spaces. However, the utility of this particular representation is that for those states with bounded or limited correlations it is often extremely efficient (in n) to extract local properties, such as expectation values of local operators.

The utility of the FCS representation as a means to calculate local properties of 1D quantum lattice systems has been spectacularly demonstrated by the development of the *density matrix renormalisation group* (DMRG). (See [5] and references therein for a description of the DMRG and related algorithms.) The DMRG provides an apparently efficient computational recipe to obtain an approximation to the ground state and low-energy eigenstates for 1D quan-

tum lattice systems as FCS vectors. The DMRG is an extremely flexible method and has been recently extended to apply to a diverse number of situations, such as the calculation of short-time dynamics [6, 7], dissipation [8, 9], disordered systems [10], eigenstates with definite momentum [11], and, recently, higher dimensions [3].

Perhaps one of the most exciting recent results in the study of the DMRG has been the development of an algorithm to simulate the real-time dynamics of 1D quantum spin systems [6, 7, 12]. The efficiency of this algorithm is predicated on the condition that the dynamics of the spin system do not create too much long-range quantum entanglement [6, 7]. While it appears that, in practice, this condition is always fulfilled for small times, it is currently unclear if it is true for *all* 1D local quantum spin systems.

There are at least two reasons why it is interesting to study the theoretical worst-case computational costs of the time-dependent DMRG. The first is that the computational complexity of the DMRG and related algorithms is currently unknown except for when applied to a handful of singular integrable models [13]. An assessment of the theoretical worst-case computational complexity of the DMRG in any other circumstance would allow one to certify *a priori* the accuracy of the DMRG versus computational cost. The second reason is related to computational power of quantum computers (see [14] for a detailed description of quantum computation and a number of quantum algorithms including quantum simulation algorithms). The time-dependent DMRG provides a way to simulate quantum computers running quantum algorithms. A careful theoretical worst-case complexity analysis would potentially give us an insight into what quantum computations can and can't be simulated efficiently on a classical computer.

The most naive way to study the computational complexity of the time-dependent DMRG is to directly study the storage costs of representing the propagator e^{itH} when it is approximated by the Lie-Trotter expansion $e^{itH} \approx (e^{i\frac{t}{m}A}e^{i\frac{t}{m}B})^m$, for some large m [23]. Unfortunately, however, a careful analysis of the error scaling with m for
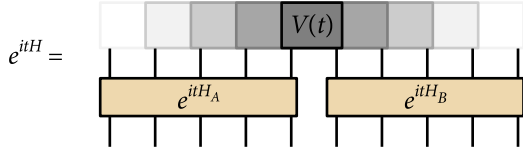
FIG. 1: Decomposing the propagator: for a given time t the propagator e^{itH} may be written as a product of $e^{it(H_A+H_B)}$ and $V(t)$, where H_A (respectively, H_B) is the hamiltonian with interaction terms only between spins in region A (respectively, between spins in region B) and $V(t)$ is a unitary operator which "patches up" the error due to approximating e^{itH} with $e^{it(H_A+H_B)}$. Because of the UV cutoff given by the lattice, information propagation in quantum spin systems is limited by an effective "speed of light". Hence the unitary $V(t)$ interacts spins in A with spins in B successively weaker further from the boundary between A and B.
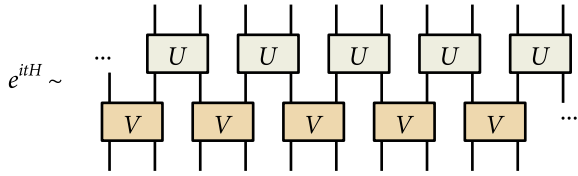

FIG. 2: The approximate quantum cellular automata decomposition for e^{itH} for time t. Each of the unitary operators U and V acts on at most $c_0|t|$ spins, where c_0 is a constant.

this representation shows that the worst-case storage cost might be exponential, even for $|t|$ which scales as a constant with n. This, in turn, implies that quantum circuits simulating 1D dynamics using the Lie-Trotter expansion have a depth that scales at least linearly with n. If we want to simulate such methods efficiently we need a more sophisticated technique to obtain a representation for the propagator.

In this Letter we show that the propagator e^{itH} for an *arbitrary* 1D quantum system is well-approximated by a finitely correlated state vector in the Hilbert space of operators using resources that scale polynomially with n and exponentially with $|t|$. Because our proof is constructive we obtain an efficient algorithm, closely related to the DMRG, to obtain this representation.

The argument we describe in this Letter can be understood by appealing to the following physical intuition. The dynamics of any 1D quantum spin system are constrained by the ultraviolet cutoff induced by the lattice spacing between the spins. This cutoff induces a bound on the speed at which information can propagate in such systems, an intuition which is precisely quantified by the *Lieb-Robinson bound* [15]. We exploit this bound on information propagation to provide two different decompositions of the propagator e^{itH}. In the first decomposition we partition the chain into two contiguous pieces A and B and approximate the dynamics e^{itH} by $e^{it(H_A+H_B)}$, where H_A is the hamiltonian which includes interaction terms only between spins

in A (and similarly for H_B). Obviously this approximation is not exact: at the cut point between A and B there will be substantial errors. However, as a consequence of the bound on information propagation, the difference between the way e^{itH} and $e^{it(H_A+H_B)}$ act on spins far from the cut will become small (information about the cut doesn't have time to propagate too far away). We can patch up the difference between the two propagators by introducing a new unitary operator $V(t)$ which acts across the boundary: $e^{itH} = e^{it(H_A+H_B)}V(t)$. The Lieb-Robinson bound then tells us that $V(t)$ acts progressively weaker on spins far from the cut (see Fig. 1 for discussion and illustration of this). This, in turn, allows us to approximate $V(t)$ with a unitary $V'(t)$ which acts nontrivially only on a *finite* number of spins Ω around the boundary. If $|\Omega|$ is bigger than $|t|$ then this approximation improves exponentially fast in $|\Omega|$.

We obtain the second decomposition for e^{itH} by first fixing t and then moving along the chain $\mathcal{C}$ and introducing a cut after approximately $|t|$ spins (which we call Λ_1) and then patching it up with a unitary $V_1(t)$ which acts nontrivially only on a finite number of spins across the boundary (this is the unitary constructed in the previous paragraph). Thus we have $e^{itH} \sim V_1(t)e^{itH_{\Lambda_1}} \otimes e^{itH_{\mathcal{C}\backslash\Lambda_1}}$. Then we recursively apply this procedure to $e^{itH_{\mathcal{C}\backslash\Lambda_1}}$ until we arrive at the approximate decomposition illustrated in Fig. 2.

We will, for the sake of clarity, describe our results mainly for a finite chain $\mathcal{C}$ of n distinguishable spin-$1/2$ particles. The family H of local hamiltonians we focus on (which implicitly depends on n) is defined by $H = \sum_{j=0}^{n-2} h_j$, where h_j acts nontrivially only on spins j and $j+1$. We set the energy scale by assuming that $\|h_j\|$ scales as a constant with n for all $j = 0, 1, \ldots, n-1$, where $\|\cdot\|$ denotes the operator norm. The interaction terms h_j may depend on time: $h_j = h_j(t)$. We can easily accommodate next-nearest neighbour interactions etc. by blocking sites and thinking of the blocks as new (larger) spins. However this can only be done a constant number of times: the quality of our approximation will decrease exponentially with the number of such blockings. We do not assume translational invariance.

The crucial idea underlying our approach is that a good approximation to the propagator e^{itH} for a local 1D quantum spin lattice system can be obtained and stored efficiently (i.e. with polynomial resources in n) with a classical computer for $|t| \leq c \log(n)$, where c is some constant. The way we do this is to use a specific representation for the approximation, namely as a *finitely correlated state vector*. What we mean by this is that we represent an operator W in the following fashion

$$W = \sum_{\boldsymbol{\alpha}\in Q_n} \mathbf{A}^{\alpha_0}\mathbf{A}^{\alpha_1}\cdots\mathbf{A}^{\alpha_{n-1}}\sigma^{\alpha_0}\otimes\sigma^{\alpha_1}\otimes\cdots\otimes\sigma^{\alpha_{n-1}},$$

(1)

where $Q_n = \{0,1,2,3\}^{\times n}$, $\mathbf{A}^{\alpha_0}$ (respectively, $\mathbf{A}^{\alpha_{n-1}}$) are a collection of four row vectors of size D_0 (respectively,

four column vectors of size C_{n-1}), $\mathbf{A}^{\alpha_j}$ are four $C_j \times D_j$ sized matrices, for $1 \leq j < n-1$, and σ^α is the vector of Pauli operators. Note that $C_{j+1} = D_j$. The dimensions C_j and D_j are called the auxiliary dimensions for site j. It is clear that if the sizes of the auxiliary dimensions are bounded by polynomials in n, i.e. if $C_j \leq \text{poly}(n)$ and $D_j \leq \text{poly}(n)$, then the operator W can be stored with polynomial resources in n. Also note that all operators can be represented exactly as in Eq. (1) by taking the auxiliary dimensions to be large enough: $C_j = D_j = 2^n$ suffices [1, 16].

We begin by showing how to obtain an approximate decomposition of the propagator e^{itH} as a product

$$e^{itH} = \left(\bigotimes_{j=0}^{n/|\Omega|-1} U_{\Omega_j}(t) \right) \left(\bigotimes_{j=0}^{n/|\Omega|} V_{\Omega_j'}(t) \right) + O(\epsilon), \quad (2)$$

where we have two partitions $\mathcal{P}_1$ and $\mathcal{P}_2$ of the chain $\mathcal{C}$ into $n/|\Omega|$ (respectively $n/|\Omega| + 1$) contiguous blocks of $\leq |\Omega|$ spins. The first set is denoted $\mathcal{P}_1 = \{\Omega_j\}$. The second set $\mathcal{P}_2 = \{\Omega_j'\}$ is the set of blocks which are just translates of those in $\mathcal{P}_1$ by $|\Omega|/2$ sites [24]. The operators U_{Ω_j} (respectively, $V_{\Omega_j'}$) are unitary operators which act nontrivially only on Ω_j (respectively, Ω_j'). We call such a decomposition an *approximate quantum cellular automata decomposition* (or, simply, an ϵ-QCA decomposition) because e^{itH} is exactly a Margolus-partitioned QCA update rule (see [17] for a description of QCA's). Then we show that an ϵ-QCA decomposition implies that e^{itH} is well-approximated by a FCS vector with auxiliary dimension $2^{|\Omega|}$. To reduce the error to ϵ we require $|\Omega| \geq c_0|t| + c_1 \log(n/\epsilon)$, where c_0 and c_1 are constants. This decomposition is illustrated in Fig. 2.

Consider the unitary operator

$$V(t) = (e^{-itH_{\mathcal{C}\backslash\Lambda}} \otimes e^{-itH_\Lambda})e^{itH}. \quad (3)$$

As we described in the introduction, for small $|t|$, and for sites far enough away from the boundary $\partial\Lambda$ between $\mathcal{C} \backslash \Lambda$ and Λ, this operator ought to be close to the identity. Therefore we argue that, as an operator, $V(t)$ ought to be expressible as $V(t) \approx \mathbb{I}_{\mathcal{C}\backslash\Omega} \otimes V_\Omega'(t)$.

To quantify this statement we study the differential equation that $V(t)$ satisfies:

$$\frac{dV(t)}{dt} = ie^{-it(H-h_I)} h_I e^{itH} = iV(t)\tau_t^H(h_I), \quad (4)$$

where h_I is the interaction term that bridges the left- and right-hand side of the chain, and $\tau_t^B(A) = e^{-itB} A e^{itB}$. Thus we see that $V(t)$ is generated by time-dependent unitary dynamics due to the effective hamiltonian $L(t) = \tau_t^H(h_I)$, and we write

$$V(t) = \mathcal{T} e^{i \int_0^t L(s)\,ds}, \quad (5)$$

where $\mathcal{T}$ denotes time-ordering.

The time-dependent effective hamiltonian $L(t)$, and hence $V(t)$, acts nontrivially on all of the sites in the chain. We now show that, for small $|t|$, $L(t)$ may be well-approximated by an operator which acts nontrivially on only a handful of sites near the boundary $\partial\Lambda$ between the left- and right-hand sides of the chain. To do this, we construct the following approximation to $L(t)$:

$$L'(t) = \tau_t^{H_\Omega}(h_I), \quad (6)$$

where Ω is a contiguous block of sites centred on $\partial\Lambda$, and H_Ω contains only those interaction terms h_j in H which interact only spins contained in Ω. We now show that, for small enough $|t|$ and large enough Ω containing H_I, $\|L(t) - L'(t)\| < \epsilon$, for some prespecified ϵ.

To show that $L'(t)$ is a good approximation to $L(t)$ we must establish that $\|\tau_t^H(h_I) - \tau_t^{H_\Omega}(h_I)\|$ is small. A bound on such a quantity is known as a *Lieb-Robinson bound* [15, 18, 19, 20] (see [21] for a simple direct proof). The strongest (and easiest to prove) such bound reads

$$\|\tau_t^H(h_I) - \tau_t^{H_\Omega}(h_I)\| \leq \sum_{l=|\Omega|}^\infty \delta_l |t|^l / l! \leq \omega e^{\kappa|t|} e^{-\mu|\Omega|},$$

where $\delta_l = \|h_I\| 2^l \|h\|^l$, $\|h\| = \max_j \|h_j\|$, and κ, μ, and ω are constants. Thus we find

$$\|L(t) - L'(t)\| = \omega e^{\kappa|t|} e^{-\mu|\Omega|}. \quad (7)$$

In this way we see that we can reduce the operator norm difference between $L(t)$ and $L'(t)$ exponentially fast in the size $|\Omega|$ of the region Ω.

We now define a new unitary operator $V'(t)$ — which is meant to approximate $V(t)$ — as the unitary operator generated by the time-dependent hamiltonian $L'(t)$:

$$\frac{dV'(t)}{dt} = iV'(t)L'(t). \quad (8)$$

Because $L'(t)$ acts nontrivially only on Ω, $V'(t)$ is a unitary operator which acts nontrivially only on Ω and it acts as an identity elsewhere. In order to see how accurate $V(t)$ is as an approximation to $V'(t)$ we now bound the error $\|V(t) - V'(t)\|$.

To show that $V(t)$ and $V'(t)$ are close for some time period we integrate the differential equations (4) and (8). We do this by making use of the Lie-Trotter expansion

$$V(t) = \lim_{m\to\infty} \prod_{j=0}^{m-1} e^{iL(\frac{jt}{m})\frac{t}{m}} \quad (9)$$

$$V'(t) = \lim_{m\to\infty} \prod_{j=0}^{m-1} e^{iL'(\frac{jt}{m})\frac{t}{m}}, \quad (10)$$

applying the triangle inequality several times, and taking the limit $m \to \infty$. This gives us the fundamental estimate

$$\|V(t) - V'(t)\| \leq \int_0^{|t|} \|L(s) - L'(s)\| ds. \quad (11)$$

Substituting (7) and redefining constants gives us

$$\|V(t) - V'(t)\| \leq \omega e^{\kappa|t|} e^{-\mu|\Omega|}, \quad (12)$$

where ω, κ, and μ are constants independent of n.

Our final result is now the following. Rearranging (3) and using the estimate (12) gives us

$$e^{itH} = (e^{itH_{C\backslash\Lambda}} \otimes e^{itH_\Lambda})V'(t) + \epsilon, \qquad (13)$$

where $V'(t)$ acts nontrivially only on a contiguous block Ω of spins of size $|\Omega|$. Iterating this procedure by cutting Λ into two pieces etc. give us the final ϵ-QCA decomposition

$$e^{itH} = \left(\bigotimes_{j=0}^{n/|\Omega|-1} U_{\Omega_j}(t)\right)\left(\bigotimes_{j=0}^{n/|\Omega|} V_{\Omega'_j}(t)\right) + O(\epsilon), \quad (14)$$

where $|\Omega| = O(c_0|t| + c_1\log(n/\epsilon))$, for some constants c_0 and c_1.

It is now relatively straightforward to show that an ϵ-QCA decomposition gives rise to an efficient FCS vector representation once we recognise that the expression

$$\mathcal{U}(t) = \left(\bigotimes_{j=0}^{n/|\Omega|-1} U_{\Omega_j}(t)\right) \qquad (15)$$

is a FCS vector with auxiliary dimension $2^{|\Omega|}$ The way to see this is to note that, in the standard operator basis,

$$U(t) = \prod_{j=0}^{n/|\Omega|-1}\left(\sum_{\mathbf{k}_j \in Q_{|\Omega|}} c_{\mathbf{k}_j}(t)\sigma_{\Omega_j}^{\mathbf{k}_j}\right)$$
$$= \sum_{\mathbf{k}} c_{\mathbf{k}_0}(t)c_{\mathbf{k}_1}(t)\cdots c_{\mathbf{k}_{n/|\Omega|-1}}(t)\sigma^{\mathbf{k}}, \quad (16)$$

which is a FCS vector representation with maximum auxiliary dimension $2^{|\Omega|}$.

Given that

$$\mathcal{V}(t) = \left(\bigotimes_{j=0}^{n/|\Omega|} V_{\Omega'_j}(t)\right) \qquad (17)$$

is also expressible exactly as a FCS with maximum auxiliary dimension $2^{|\Omega|}$ and using the result that the product of two FCS vector operators with maximum auxiliary dimensions D_1 and D_2 admits a FCS vector expression with maximum auxiliary dimensions $D_1 D_2$ we obtain the final result that our approximation $V'(t) = \mathcal{U}(t)\mathcal{V}(t)$ to $V(t)$ is expressible exactly as a FCS with maximum auxiliary dimension $\leq 2^{2|\Omega|}$. If $|t|$ scales as a constant, or logarithmically, with n then we learn that the FCS representation requires only polynomial resources in n.

We have shown how the propagator e^{itH} for a 1D system of quantum spins can be efficiently obtained and represented using a classical computer. There are many consequences of this representation. The first and most obvious is that the time-dependent DMRG will, in the theoretical worst case, require only polynomial computational resources to simulate time evolution for constant times.

I would especially like to thank to thank Ignacio Cirac, Toby Cubitt, Jens Eisert, Henry Haselgrove, Nick Jones,

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[22] It is worth noting that any quantum state can be written as a FCS, however, the more correlated the state, the more expensive (in terms of memory usage) this becomes.
[23] The Lie-Trotter expansion is the key ingredient exploited to simulate dynamics in the time-dependent DMRG.
[24] At each end of the chain the second partition $\mathcal{P}_2$ has a block of size $|\Omega|/2$